Full wwPDB X-ray Structure Validation Report ⓘ

Nov 15, 2023 – 12:55 AM JST

PDB ID	:	6ILZ
Title	:	Crystal structure of PKCiota in complex with inhibitor
Authors	:	Baburajendran, N.; Hill, J.
Deposited on	:	2018-10-21
Resolution	:	3.26 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

The following versions of software and data (see references ⓘ) were used in the production of this report:

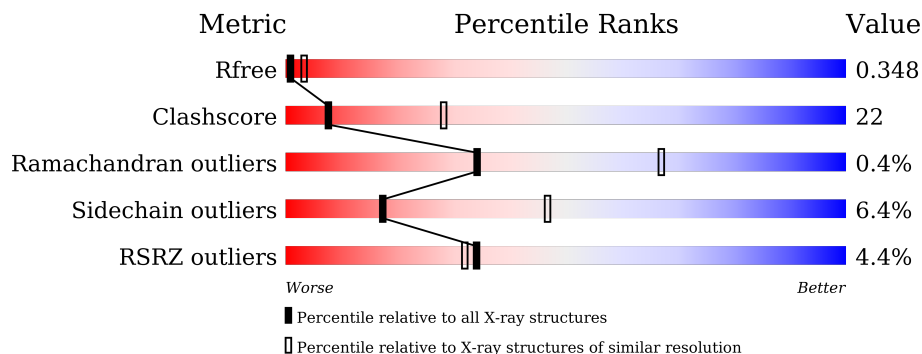|		
MolProbity	:	4.02b-467
Mogul	:	1.8.5 (274361), CSD as541be (2020)
Xtriage (Phenix)	:	1.13
EDS	:	2.36
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
Refmac	:	5.8.0158
CCP4	:	7.0.044 (Gargrove)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.36

1 Overall quality at a glance ⓘ

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.26 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.

Metric	Percentile Ranks	Value
Rfree		0.348
Clashscore		22
Ramachandran outliers		0.4%
Sidechain outliers		6.4%
RSRZ outliers		4.4%

Worse   *Better*

▌Percentile relative to all X-ray structures

▯Percentile relative to X-ray structures of similar resolution

Metric	Whole archive (#Entries)	Similar resolution (#Entries, resolution range(Å))
R_{free}	130704	1191 (3.30-3.22)
Clashscore	141614	1251 (3.30-3.22)
Ramachandran outliers	138981	1229 (3.30-3.22)
Sidechain outliers	138945	1228 (3.30-3.22)
RSRZ outliers	127900	1154 (3.30-3.22)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments of the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	345	3% — 53% / 38% / • 7%
1	C	345	3% — 61% / 28% / • 8%
1	E	345	5% — 51% / 37% / • 8%
1	G	345	5% — 48% / 40% / • 9%

2 Entry composition (i)

There are 2 unique types of molecules in this entry. The entry contains 9673 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.
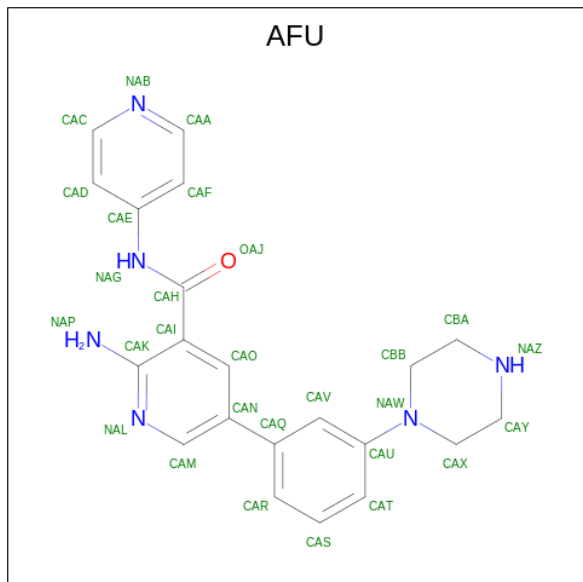
- Molecule 1 is a protein called Protein kinase C iota type.

Mol	Chain	Residues	Atoms						ZeroOcc	AltConf	Trace
1	A	320	Total	C	N	O	P	S	0	0	0
			2445	1559	414	457	2	13			
1	C	317	Total	C	N	O	P	S	0	0	0
			2389	1530	406	439	2	12			
1	E	316	Total	C	N	O	P	S	0	0	0
			2363	1512	397	439	2	13			
1	G	315	Total	C	N	O	P	S	0	0	0
			2364	1514	390	445	2	13			

There are 20 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	244	GLY	-	expression tag	UNP P41743
A	245	ALA	-	expression tag	UNP P41743
A	246	MET	-	expression tag	UNP P41743
A	247	ASP	-	expression tag	UNP P41743
A	248	PRO	-	expression tag	UNP P41743
C	244	GLY	-	expression tag	UNP P41743
C	245	ALA	-	expression tag	UNP P41743
C	246	MET	-	expression tag	UNP P41743
C	247	ASP	-	expression tag	UNP P41743
C	248	PRO	-	expression tag	UNP P41743
E	244	GLY	-	expression tag	UNP P41743
E	245	ALA	-	expression tag	UNP P41743
E	246	MET	-	expression tag	UNP P41743
E	247	ASP	-	expression tag	UNP P41743
E	248	PRO	-	expression tag	UNP P41743
G	244	GLY	-	expression tag	UNP P41743
G	245	ALA	-	expression tag	UNP P41743
G	246	MET	-	expression tag	UNP P41743
G	247	ASP	-	expression tag	UNP P41743
G	248	PRO	-	expression tag	UNP P41743

- Molecule 2 is 2-amino-5-[3-(piperazin-1-yl)phenyl]-N-(pyridin-4-yl)pyridine-3-carboxamide (three-letter code: AFU) (formula: $C_{21}H_{22}N_6O$).


| Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	1	Total	C	N	O	0	0
			28	21	6	1		
2	C	1	Total	C	N	O	0	0
			28	21	6	1		
2	E	1	Total	C	N	O	0	0
			28	21	6	1		
2	G	1	Total	C	N	O	0	0
			28	21	6	1		

3 Residue-property plots ⓘ

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red dot above a residue indicates a poor fit to the electron density (RSRZ > 2). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.
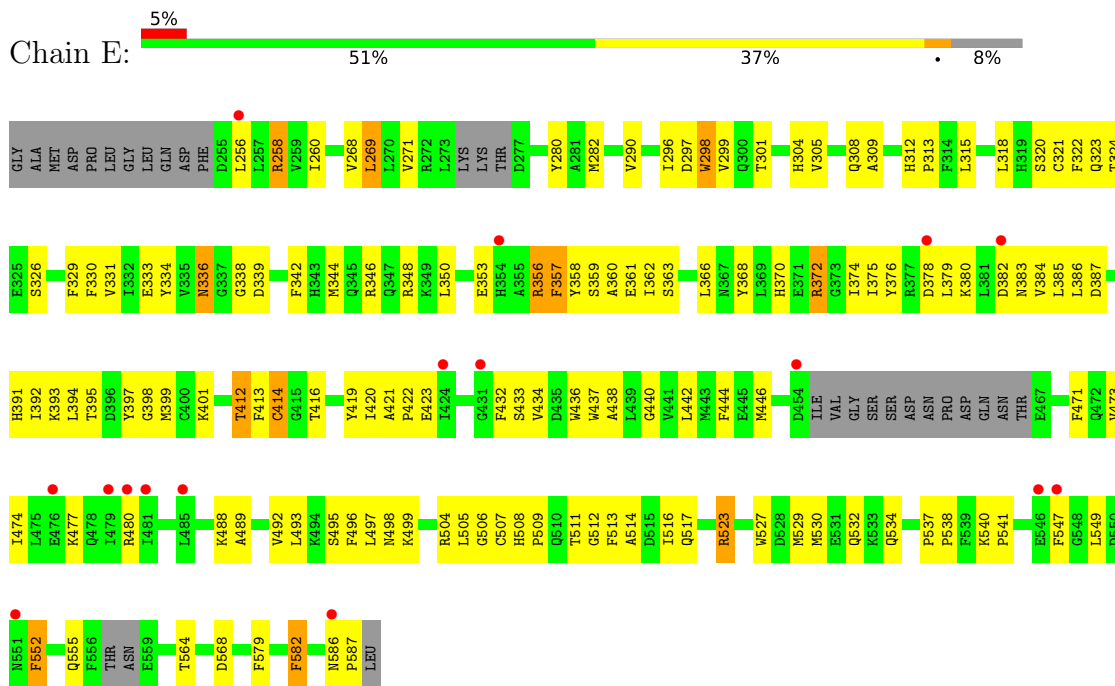
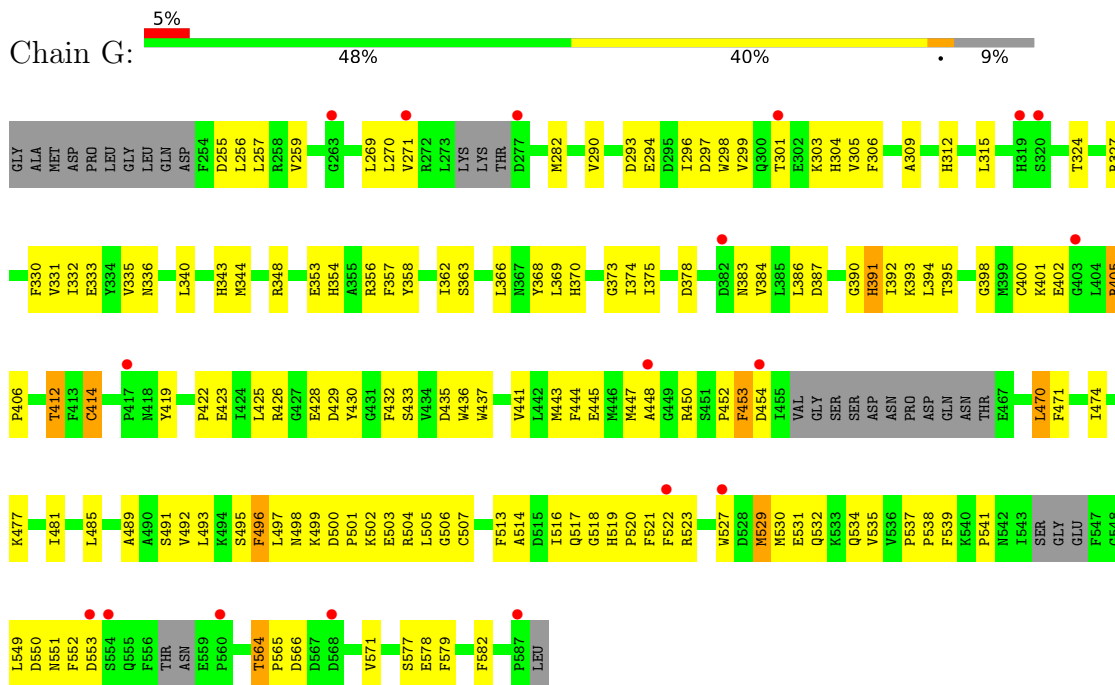- Molecule 1: Protein kinase C iota type
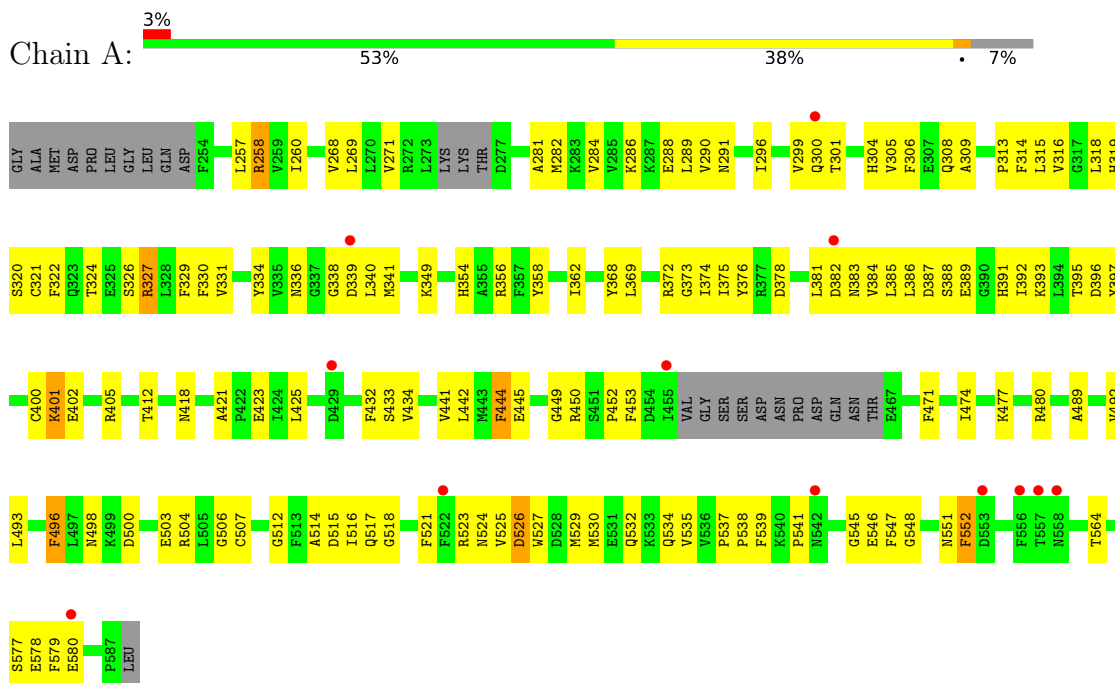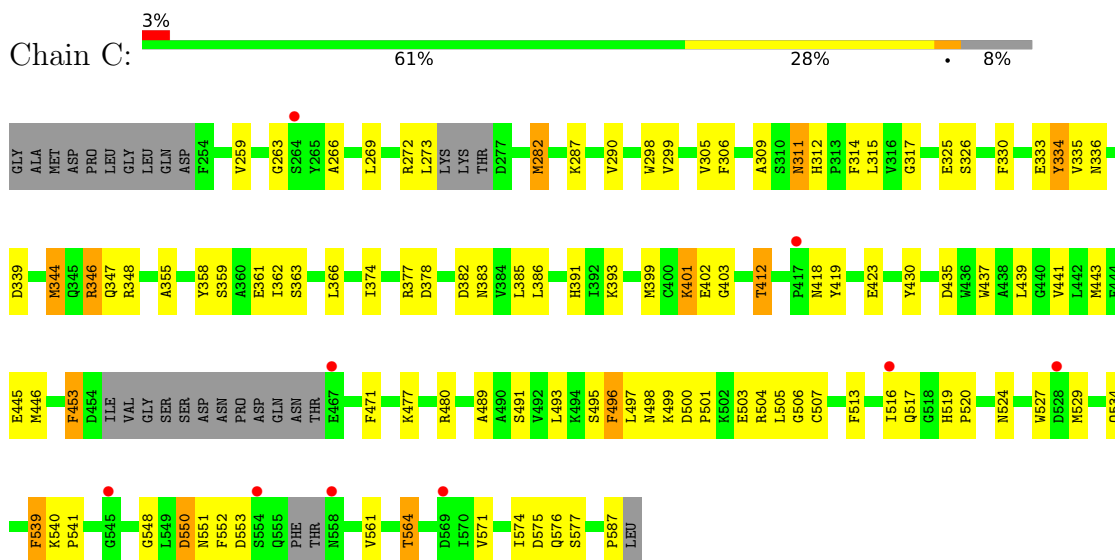
- Molecule 1: Protein kinase C iota type

• Molecule 1: Protein kinase C iota type

Chain E:

• Molecule 1: Protein kinase C iota type

Chain G:

4 Data and refinement statistics ⓘ

Property	Value	Source
Space group	P 1 21 1	Depositor
Cell constants a, b, c, α, β, γ	87.87Å 87.63Å 105.18Å 90.00° 114.69° 90.00°	Depositor
Resolution (Å)	51.58 – 3.26 51.58 – 3.26	Depositor EDS
% Data completeness (in resolution range)	97.1 (51.58-3.26) 96.0 (51.58-3.26)	Depositor EDS
R_{merge}	0.08	Depositor
R_{sym}	(Not available)	Depositor
$<I/\sigma(I)>$ [1]	2.96 (at 3.26Å)	Xtriage
Refinement program	PHENIX 1.14_3260	Depositor
R, R_{free}	0.306 , 0.348 0.305 , 0.348	Depositor DCC
R_{free} test set	1998 reflections (9.01%)	wwPDB-VP
Wilson B-factor (Å^2)	46.4	Xtriage
Anisotropy	0.202	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.33 , 14.3	EDS
L-test for twinning[2]	$<|L|>$ = 0.41, $<L^2>$ = 0.23	Xtriage
Estimated twinning fraction	0.238 for h,-k,-h-l	Xtriage
F_o,F_c correlation	0.74	EDS
Total number of atoms	9673	wwPDB-VP
Average B, all atoms (Å^2)	32.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 6.88% of the height of the origin peak. No significant pseudotranslation is detected.*

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[1]Intensities estimated from amplitudes.
[2]Theoretical values of $<|L|>$, $<L^2>$ for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 0.2 for perfectly twinned datasets.

5 Model quality ⓘ

5.1 Standard geometry ⓘ

Bond lengths and bond angles in the following residue types are not validated in this section: AFU, TPO

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$|Z|$ >5	RMSZ	#$|Z|$ >5
1	A	0.42	0/2477	0.57	0/3356
1	C	0.44	1/2421 (0.0%)	0.57	1/3283 (0.0%)
1	E	0.39	0/2393	0.55	0/3248
1	G	0.44	1/2394 (0.0%)	0.57	0/3250
All	All	0.42	2/9685 (0.0%)	0.56	1/13137 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	470	LEU	CG-CD1	-5.51	1.31	1.51
1	C	496	PHE	CE2-CZ	-5.12	1.27	1.37

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	550	ASP	CB-CG-OD2	6.13	123.81	118.30

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2445	0	2249	102	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	C	2389	0	2163	83	0
1	E	2363	0	2136	97	0
1	G	2364	0	2129	119	0
2	A	28	0	0	2	0
2	C	28	0	0	3	0
2	E	28	0	0	2	0
2	G	28	0	0	2	0
All	All	9673	0	8677	403	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 22.

All (403) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:378:ASP:O	1:C:383:ASN:ND2	2.02	0.92
1:E:378:ASP:O	1:E:383:ASN:ND2	2.06	0.89
1:A:286:LYS:HE2	1:A:327:ARG:HH21	1.38	0.88
1:A:385:LEU:HD23	1:A:552:PHE:HZ	1.39	0.87
1:G:532:GLN:HB2	1:G:534:GLN:NE2	1.90	0.86
1:A:313:PRO:O	1:A:393:LYS:NZ	2.09	0.85
1:G:532:GLN:HB2	1:G:534:GLN:HE22	1.40	0.84
1:E:323:GLN:NE2	1:E:579:PHE:O	2.12	0.83
1:G:378:ASP:O	1:G:383:ASN:ND2	2.13	0.81
1:G:566:ASP:HB2	1:G:571:VAL:HG21	1.63	0.81
1:A:290:VAL:HG11	1:A:299:VAL:HG13	1.62	0.80
1:G:529:MET:HG2	1:G:534:GLN:HB3	1.62	0.80
1:A:304:HIS:O	1:A:308:GLN:NE2	2.13	0.80
1:A:498:ASN:ND2	1:A:503:GLU:OE1	2.15	0.80
1:G:256:LEU:HD22	1:G:271:VAL:HG12	1.64	0.79
1:E:313:PRO:O	1:E:393:LYS:NZ	2.16	0.79
1:A:291:ASN:ND2	1:A:578:GLU:OE1	2.15	0.78
1:E:280:TYR:OH	1:E:333:GLU:OE2	2.00	0.78
1:E:318:LEU:HD12	1:E:331:VAL:O	1.85	0.77
1:G:492:VAL:HG21	1:G:522:PHE:HE2	1.49	0.77
1:A:301:THR:HG23	1:A:402:GLU:HG2	1.67	0.76
1:E:376:TYR:OH	1:E:395:THR:O	2.02	0.76
1:G:423:GLU:OE2	1:G:504:ARG:NH2	2.19	0.76
1:G:366:LEU:O	1:G:370:HIS:ND1	2.20	0.75
1:A:381:LEU:HD12	1:A:442:LEU:HD12	1.67	0.74
1:G:259:VAL:HG22	1:G:269:LEU:HD21	1.68	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:529:MET:HG2	1:G:534:GLN:CB	2.18	0.73
1:A:286:LYS:HE2	1:A:327:ARG:NH2	2.03	0.73
1:C:441:VAL:O	1:C:445:GLU:HG3	1.88	0.73
1:A:545:GLY:O	1:A:548:GLY:N	2.21	0.73
1:G:333:GLU:OE1	1:G:393:LYS:NZ	2.22	0.72
1:G:256:LEU:CD2	1:G:271:VAL:HG12	2.19	0.72
1:G:401:LYS:NZ	1:G:414:CYS:SG	2.60	0.71
1:G:297:ASP:O	1:G:301:THR:OG1	2.08	0.71
1:A:423:GLU:OE2	1:A:433:SER:OG	2.09	0.71
1:E:350:LEU:N	1:E:446:MET:O	2.20	0.71
1:A:336:ASN:OD1	1:A:388:SER:N	2.24	0.70
1:G:312:HIS:NE2	1:G:531:GLU:OE1	2.23	0.70
1:A:358:TYR:O	1:A:362:ILE:HG13	1.92	0.70
1:C:385:LEU:O	1:C:393:LYS:N	2.25	0.69
1:C:423:GLU:OE2	1:C:504:ARG:NH2	2.25	0.69
1:G:453:PHE:CZ	1:G:474:ILE:HG23	2.28	0.69
1:A:515:ASP:OD2	1:A:515:ASP:N	2.24	0.69
1:G:505:LEU:HG	1:G:516:ILE:HG22	1.75	0.69
1:E:423:GLU:OE2	1:E:433:SER:OG	2.06	0.69
1:C:500:ASP:HB3	1:C:503:GLU:HB3	1.75	0.69
1:E:529:MET:HG3	1:E:534:GLN:HB2	1.75	0.69
1:E:420:ILE:O	1:E:437:TRP:NE1	2.26	0.68
1:A:385:LEU:N	1:A:393:LYS:O	2.26	0.68
1:A:389:GLU:O	1:A:537:PRO:HG3	1.94	0.68
2:C:601:AFU:OAJ	2:C:601:AFU:NAP	2.24	0.67
1:G:470:LEU:HD12	1:G:471:PHE:N	2.09	0.67
1:G:517:GLN:HG2	1:G:527:TRP:CE2	2.30	0.66
1:C:399:MET:O	1:C:401:LYS:NZ	2.18	0.66
1:C:314:PHE:O	1:C:393:LYS:HA	1.96	0.66
1:G:450:ARG:NH2	1:G:454:ASP:OD1	2.29	0.66
1:A:378:ASP:O	1:A:383:ASN:ND2	2.29	0.66
1:G:441:VAL:O	1:G:445:GLU:HG3	1.96	0.66
1:G:523:ARG:NE	1:G:523:ARG:O	2.29	0.65
1:G:532:GLN:CB	1:G:534:GLN:HE22	2.10	0.65
1:G:519:HIS:CG	1:G:520:PRO:HD2	2.32	0.65
1:C:336:ASN:HA	1:C:552:PHE:HZ	1.61	0.65
1:A:300:GLN:O	1:A:304:HIS:ND1	2.29	0.65
1:A:318:LEU:HD21	1:A:321:CYS:SG	2.37	0.64
1:E:305:VAL:O	1:E:309:ALA:N	2.31	0.64
1:E:256:LEU:HB3	1:E:269:LEU:HD12	1.80	0.64
1:E:322:PHE:HB3	1:E:329:PHE:HB2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:260:ILE:O	1:E:268:VAL:HB	1.97	0.64
1:E:540:LYS:HG2	1:E:541:PRO:HD2	1.80	0.64
1:E:318:LEU:HD21	1:E:321:CYS:SG	2.37	0.63
1:C:575:ASP:OD2	1:C:577:SER:OG	2.10	0.63
1:A:444:PHE:CD1	1:A:452:PRO:HB3	2.33	0.63
1:C:269:LEU:HD11	1:C:282:MET:HE3	1.79	0.63
2:A:601:AFU:OAJ	2:A:601:AFU:NAP	2.24	0.63
1:A:506:GLY:HA3	1:A:516:ILE:HD11	1.79	0.62
1:C:496:PHE:HZ	1:C:516:ILE:CD1	2.12	0.62
1:A:423:GLU:OE2	1:A:504:ARG:NH1	2.24	0.62
1:C:358:TYR:O	1:C:362:ILE:HG13	1.97	0.62
1:G:470:LEU:O	1:G:474:ILE:HG13	1.99	0.62
1:A:362:ILE:HG12	1:A:392:ILE:HD13	1.81	0.62
1:E:366:LEU:O	1:E:370:HIS:ND1	2.33	0.62
1:A:316:VAL:N	1:A:397:TYR:OH	2.33	0.62
1:C:334:TYR:OH	1:C:548:GLY:O	2.17	0.62
1:E:358:TYR:O	1:E:362:ILE:HG13	2.00	0.62
1:G:500:ASP:HB3	1:G:503:GLU:HB3	1.82	0.62
1:C:259:VAL:HG23	1:C:561:VAL:HA	1.82	0.61
1:G:343:HIS:CD2	1:G:386:LEU:HD11	2.35	0.61
1:A:480:ARG:HH21	1:G:577:SER:HB2	1.65	0.61
1:C:564:TPO:P	1:C:564:TPO:H	2.23	0.61
1:E:359:SER:O	1:E:363:SER:OG	2.19	0.60
1:G:290:VAL:HG11	1:G:299:VAL:HG13	1.83	0.60
1:E:256:LEU:HD13	1:E:269:LEU:HD11	1.84	0.60
1:E:380:LYS:HD3	1:E:416:THR:HG21	1.83	0.60
1:A:369:LEU:O	1:A:373:GLY:N	2.32	0.59
1:C:496:PHE:CZ	1:C:516:ILE:HD12	2.36	0.59
1:C:498:ASN:ND2	1:C:503:GLU:OE1	2.34	0.59
1:E:387:ASP:O	1:E:541:PRO:HG3	2.02	0.59
1:E:508:HIS:CE1	1:E:511:THR:H	2.21	0.59
2:E:601:AFU:NAP	2:E:601:AFU:OAJ	2.31	0.59
1:E:290:VAL:HG11	1:E:299:VAL:HG13	1.84	0.59
1:G:305:VAL:HG22	1:G:374:ILE:HG21	1.83	0.59
1:G:357:PHE:CD2	1:G:538:PRO:HD3	2.37	0.59
1:G:493:LEU:O	1:G:497:LEU:HB2	2.02	0.59
1:C:269:LEU:CD1	1:C:282:MET:HB3	2.33	0.59
1:E:442:LEU:O	1:E:446:MET:HG3	2.03	0.59
1:C:269:LEU:HD12	1:C:269:LEU:O	2.03	0.58
1:G:422:PRO:O	1:G:426:ARG:N	2.28	0.58
1:G:437:TRP:CZ3	1:G:497:LEU:HD23	2.38	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:359:SER:O	1:C:363:SER:OG	2.21	0.58
1:E:375:ILE:HG12	1:E:432:PHE:CD2	2.39	0.58
1:C:339:ASP:OD1	1:C:339:ASP:N	2.37	0.58
1:C:366:LEU:HD13	1:C:435:ASP:HB3	1.84	0.58
1:E:298:TRP:CD1	1:E:398:GLY:O	2.57	0.58
1:E:260:ILE:O	1:E:260:ILE:HG22	2.03	0.57
1:C:519:HIS:CG	1:C:520:PRO:HD2	2.39	0.57
1:G:405:ARG:CB	1:G:406:PRO:HD3	2.34	0.57
1:A:269:LEU:HD11	1:A:282:MET:HE2	1.85	0.57
1:A:386:LEU:HD23	1:A:391:HIS:O	2.03	0.57
1:A:421:ALA:HB2	1:A:434:VAL:HG23	1.86	0.57
1:G:470:LEU:HD12	1:G:471:PHE:HD1	1.70	0.57
1:C:493:LEU:O	1:C:497:LEU:HB2	2.04	0.57
1:E:308:GLN:O	1:E:368:TYR:OH	2.08	0.57
1:C:346:ARG:HG2	1:C:347:GLN:OE1	2.05	0.56
1:G:470:LEU:HD12	1:G:471:PHE:CD1	2.40	0.56
1:G:309:ALA:HB1	1:G:315:LEU:HD13	1.88	0.56
1:E:342:PHE:HE2	1:E:346:ARG:HH21	1.53	0.56
1:C:269:LEU:HD11	1:C:282:MET:HB3	1.87	0.56
1:A:334:TYR:HE2	1:A:547:PHE:O	1.89	0.56
1:E:298:TRP:HE1	1:E:398:GLY:HA2	1.71	0.56
1:A:489:ALA:O	1:A:493:LEU:HG	2.06	0.56
1:G:282:MET:HA	1:G:330:PHE:O	2.06	0.56
1:A:375:ILE:HG12	1:A:432:PHE:CD2	2.41	0.55
1:A:314:PHE:O	1:A:393:LYS:HA	2.06	0.55
1:A:327:ARG:HG3	1:A:329:PHE:CZ	2.42	0.55
1:A:349:LYS:HG2	1:A:449:GLY:HA3	1.87	0.55
1:C:477:LYS:HE2	1:C:480:ARG:HE	1.72	0.55
1:E:305:VAL:HG22	1:E:374:ILE:HD12	1.86	0.55
1:G:390:GLY:HA2	1:G:541:PRO:HD3	1.89	0.55
1:G:447:MET:HB3	1:G:485:LEU:HD21	1.88	0.55
1:E:321:CYS:HB3	1:E:582:PHE:CD2	2.42	0.54
1:A:500:ASP:HB3	1:A:503:GLU:HB3	1.88	0.54
1:A:383:ASN:HA	1:A:395:THR:HG22	1.89	0.54
1:G:491:SER:O	1:G:495:SER:OG	2.16	0.54
1:A:368:TYR:O	1:A:372:ARG:HG2	2.07	0.54
1:E:440:GLY:O	1:E:444:PHE:N	2.41	0.54
1:E:304:HIS:O	1:E:308:GLN:HG3	2.08	0.54
1:G:426:ARG:NH1	1:G:499:LYS:O	2.41	0.54
1:E:474:ILE:O	1:E:499:LYS:HE3	2.08	0.54
1:A:385:LEU:CD2	1:A:552:PHE:HZ	2.18	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:335:VAL:O	1:G:552:PHE:HZ	1.91	0.53
1:G:566:ASP:HB2	1:G:571:VAL:CG2	2.36	0.53
1:E:549:LEU:H	1:E:549:LEU:HD23	1.73	0.53
1:G:298:TRP:HE1	1:G:398:GLY:HA2	1.74	0.53
1:A:327:ARG:HG3	1:A:329:PHE:CE2	2.44	0.53
1:G:444:PHE:HE1	1:G:481:ILE:HD13	1.74	0.53
1:G:498:ASN:ND2	1:G:503:GLU:HG2	2.24	0.53
1:A:506:GLY:HA2	1:A:512:GLY:O	2.08	0.53
1:E:508:HIS:HB3	1:E:512:GLY:HA2	1.91	0.53
1:A:418:ASN:O	1:A:453:PHE:HE1	1.91	0.53
1:A:504:ARG:HB3	1:A:507:CYS:SG	2.49	0.53
1:E:508:HIS:HB3	1:E:512:GLY:CA	2.39	0.53
1:C:362:ILE:O	1:C:366:LEU:HG	2.09	0.53
1:C:529:MET:O	1:C:534:GLN:HB2	2.09	0.52
1:E:368:TYR:O	1:E:372:ARG:HG2	2.09	0.52
1:C:423:GLU:OE1	1:C:423:GLU:N	2.30	0.52
1:A:376:TYR:HE1	1:A:396:ASP:O	1.93	0.52
1:C:550:ASP:OD1	1:C:551:ASN:OD1	2.28	0.52
1:G:369:LEU:O	1:G:374:ILE:N	2.33	0.52
1:C:437:TRP:CZ2	1:C:453:PHE:CZ	2.96	0.52
1:G:530:MET:HE2	1:G:535:VAL:HG11	1.91	0.52
1:A:375:ILE:HG12	1:A:432:PHE:CE2	2.45	0.52
1:E:344:MET:O	1:E:348:ARG:HA	2.10	0.52
1:A:385:LEU:HD23	1:A:552:PHE:CZ	2.31	0.52
1:C:344:MET:O	1:C:348:ARG:HA	2.10	0.52
1:E:361:GLU:HB3	1:E:392:ILE:HD11	1.92	0.52
1:E:473:VAL:O	1:E:477:LYS:N	2.43	0.52
1:E:506:GLY:HA3	1:E:516:ILE:HD11	1.91	0.52
1:C:269:LEU:HD11	1:C:282:MET:CE	2.40	0.52
1:A:444:PHE:CE1	1:A:452:PRO:HB3	2.44	0.52
1:C:412:TPO:O	1:C:430:TYR:CE2	2.63	0.52
1:G:391:HIS:CE1	1:G:537:PRO:HG3	2.45	0.52
1:C:361:GLU:OE1	1:C:391:HIS:ND1	2.38	0.51
1:G:353:GLU:O	1:G:356:ARG:HG3	2.10	0.51
1:G:428:GLU:OE1	1:G:429:ASP:N	2.41	0.51
1:E:271:VAL:HG11	1:E:282:MET:HE2	1.92	0.51
1:E:504:ARG:HB3	1:E:507:CYS:SG	2.50	0.51
1:G:383:ASN:O	1:G:395:THR:OG1	2.27	0.51
1:E:334:TYR:HE2	1:E:336:ASN:HB3	1.75	0.51
1:E:338:GLY:HA2	1:E:552:PHE:CE1	2.45	0.51
1:A:577:SER:O	1:A:580:GLU:HB3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:356:ARG:HB2	1:A:521:PHE:HE2	1.75	0.51
1:C:386:LEU:HA	1:C:391:HIS:O	2.10	0.51
1:C:312:HIS:HB3	1:C:315:LEU:HD12	1.93	0.51
1:G:470:LEU:CD1	1:G:471:PHE:CD1	2.94	0.50
1:E:489:ALA:O	1:E:493:LEU:HG	2.11	0.50
1:C:517:GLN:HG2	1:C:527:TRP:CE2	2.47	0.50
1:C:309:ALA:HB1	1:C:315:LEU:HD13	1.93	0.50
1:G:423:GLU:HG2	1:G:501:PRO:HB3	1.94	0.50
1:G:470:LEU:HD12	1:G:471:PHE:H	1.77	0.50
1:C:504:ARG:HD2	1:C:507:CYS:SG	2.52	0.49
1:E:514:ALA:HA	1:E:517:GLN:OE1	2.12	0.49
1:A:281:ALA:HB2	1:A:334:TYR:HD1	1.78	0.49
1:E:318:LEU:HD11	1:E:320:SER:O	2.12	0.49
1:C:272:ARG:HG2	1:C:273:LEU:H	1.78	0.49
1:C:552:PHE:HB3	2:C:601:AFU:CBB	2.42	0.49
1:E:324:THR:HG23	1:E:326:SER:H	1.77	0.49
1:G:550:ASP:OD2	1:G:550:ASP:N	2.44	0.49
1:C:402:GLU:HG2	1:C:403:GLY:N	2.27	0.49
1:C:489:ALA:O	1:C:493:LEU:HG	2.12	0.49
1:G:257:LEU:CB	1:G:270:LEU:HD22	2.43	0.49
1:G:373:GLY:O	1:G:402:GLU:HA	2.13	0.49
1:A:296:ILE:HD13	1:A:579:PHE:HE2	1.78	0.49
1:E:298:TRP:NE1	1:E:398:GLY:HA2	2.28	0.49
1:G:257:LEU:HB3	1:G:270:LEU:HD22	1.95	0.49
1:G:412:TPO:O	1:G:430:TYR:OH	2.11	0.49
1:G:422:PRO:O	1:G:425:LEU:N	2.46	0.49
1:G:485:LEU:HD13	1:G:489:ALA:HB1	1.93	0.49
1:E:382:ASP:OD1	1:E:382:ASP:N	2.46	0.49
1:A:305:VAL:O	1:A:309:ALA:N	2.40	0.48
1:G:343:HIS:NE2	1:G:386:LEU:HD11	2.27	0.48
1:C:496:PHE:O	1:C:504:ARG:HD3	2.13	0.48
1:G:387:ASP:O	1:G:541:PRO:HG2	2.13	0.48
1:C:496:PHE:CE1	1:C:516:ILE:HD12	2.48	0.48
1:E:282:MET:HA	1:E:330:PHE:O	2.13	0.48
1:E:370:HIS:CD2	1:E:432:PHE:HB3	2.48	0.48
1:G:491:SER:HB3	1:G:519:HIS:CE1	2.49	0.48
1:G:340:LEU:HD21	1:G:386:LEU:HD21	1.96	0.48
1:G:358:TYR:O	1:G:362:ILE:HG13	2.14	0.48
1:C:539:PHE:HD2	1:C:540:LYS:H	1.61	0.48
1:G:426:ARG:HH12	1:G:501:PRO:HD3	1.78	0.48
1:G:549:LEU:HD12	1:G:549:LEU:H	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:394:LEU:O	1:E:397:TYR:OH	2.21	0.48
1:C:355:ALA:O	1:C:359:SER:OG	2.19	0.48
1:C:524:ASN:OD1	1:C:524:ASN:N	2.47	0.48
1:G:259:VAL:HA	1:G:269:LEU:HD23	1.94	0.48
1:A:514:ALA:O	1:A:518:GLY:N	2.43	0.47
1:A:526:ASP:HB3	1:A:529:MET:HB3	1.95	0.47
1:A:324:THR:HG23	1:A:326:SER:H	1.79	0.47
1:A:338:GLY:O	1:A:386:LEU:HB2	2.14	0.47
1:A:354:HIS:CE1	1:A:538:PRO:HB2	2.49	0.47
1:C:312:HIS:CB	1:C:315:LEU:HD12	2.44	0.47
1:C:335:VAL:HG12	1:C:386:LEU:O	2.14	0.47
1:G:312:HIS:HB3	1:G:315:LEU:HD12	1.95	0.47
1:C:505:LEU:HD12	1:C:506:GLY:H	1.79	0.47
1:E:498:ASN:O	1:E:504:ARG:NH2	2.48	0.47
1:C:317:GLY:N	1:C:333:GLU:OE2	2.48	0.47
1:A:257:LEU:HD23	1:A:547:PHE:CZ	2.50	0.47
1:A:324:THR:HG22	1:A:329:PHE:HE2	1.80	0.47
1:E:401:LYS:HZ1	1:E:412:TPO:P	2.29	0.47
1:A:336:ASN:OD1	1:A:388:SER:HB3	2.15	0.47
1:E:280:TYR:CZ	1:E:333:GLU:OE2	2.68	0.47
1:G:452:PRO:O	1:G:477:LYS:NZ	2.47	0.47
1:A:322:PHE:HE2	1:A:331:VAL:CG2	2.28	0.46
1:C:418:ASN:HB3	1:C:419:TYR:CD1	2.50	0.46
1:E:339:ASP:HA	1:E:384:VAL:O	2.15	0.46
1:A:425:LEU:HD22	1:A:471:PHE:HD1	1.80	0.46
1:E:357:PHE:CE2	1:E:537:PRO:HA	2.50	0.46
1:E:495:SER:HB2	1:E:505:LEU:HB2	1.97	0.46
1:A:530:MET:SD	1:A:535:VAL:HG11	2.55	0.46
1:G:332:ILE:HD12	2:G:601:AFU:OAJ	2.14	0.46
1:A:356:ARG:NE	1:A:525:VAL:HG13	2.30	0.46
1:A:383:ASN:HA	1:A:395:THR:CG2	2.46	0.46
1:G:293:ASP:OD2	1:G:294:GLU:N	2.48	0.46
1:G:304:HIS:ND1	1:G:402:GLU:OE2	2.46	0.46
1:G:470:LEU:CD1	1:G:471:PHE:HD1	2.29	0.46
1:G:255:ASP:OD1	1:G:255:ASP:N	2.45	0.46
1:C:282:MET:HA	1:C:330:PHE:O	2.15	0.46
1:A:340:LEU:HG	1:A:384:VAL:CG2	2.46	0.46
1:A:492:VAL:HG23	1:A:496:PHE:CD1	2.51	0.46
1:E:301:THR:O	1:E:305:VAL:HG23	2.16	0.46
1:G:324:THR:HG23	1:G:327:ARG:H	1.81	0.46
1:G:375:ILE:HG12	1:G:432:PHE:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:301:THR:O	1:A:305:VAL:HG23	2.16	0.46
1:C:471:PHE:N	1:C:471:PHE:CD1	2.84	0.46
1:G:282:MET:HG3	1:G:331:VAL:HG22	1.97	0.45
1:G:336:ASN:HA	1:G:552:PHE:CZ	2.51	0.45
1:C:263:GLY:N	1:C:266:ALA:O	2.46	0.45
1:E:258:ARG:HD2	1:E:258:ARG:HA	1.77	0.45
1:E:344:MET:CE	1:E:350:LEU:HG	2.46	0.45
1:E:353:GLU:O	1:E:356:ARG:NH2	2.50	0.45
1:G:309:ALA:HA	1:G:368:TYR:HE2	1.81	0.45
1:E:386:LEU:HA	1:E:391:HIS:O	2.16	0.45
1:G:340:LEU:HG	1:G:384:VAL:HG23	1.99	0.45
1:C:311:ASN:OD1	1:C:311:ASN:N	2.49	0.45
1:G:363:SER:HG	1:G:436:TRP:HZ3	1.59	0.45
1:A:282:MET:HA	1:A:330:PHE:O	2.16	0.45
1:A:375:ILE:O	1:A:400:CYS:HA	2.16	0.45
1:G:336:ASN:OD1	1:G:336:ASN:N	2.48	0.45
1:C:325:GLU:O	1:C:574:ILE:HD11	2.16	0.45
1:E:362:ILE:HG12	1:E:392:ILE:HD13	1.98	0.45
1:G:453:PHE:CE2	1:G:474:ILE:HG12	2.52	0.45
1:A:374:ILE:HA	1:A:401:LYS:O	2.17	0.45
1:E:586:ASN:ND2	1:E:586:ASN:O	2.50	0.45
1:G:492:VAL:HG11	1:G:521:PHE:CD2	2.51	0.45
1:G:550:ASP:OD2	1:G:551:ASN:OD1	2.35	0.45
1:A:517:GLN:HG2	1:A:527:TRP:CE2	2.51	0.45
1:C:290:VAL:HG11	1:C:299:VAL:HG13	1.99	0.44
2:G:601:AFU:OAJ	2:G:601:AFU:NAP	2.48	0.44
1:G:436:TRP:HB3	1:G:496:PHE:CD2	2.53	0.44
1:G:491:SER:HB3	1:G:519:HIS:HE1	1.83	0.44
1:C:437:TRP:HH2	1:C:499:LYS:HE2	1.81	0.44
1:G:514:ALA:O	1:G:518:GLY:N	2.50	0.44
1:A:492:VAL:O	1:A:496:PHE:HB2	2.18	0.44
1:A:532:GLN:HB2	1:A:534:GLN:HG2	1.99	0.44
1:E:360:ALA:HB1	1:E:527:TRP:CZ3	2.53	0.44
1:G:374:ILE:HA	1:G:401:LYS:O	2.18	0.44
1:E:488:LYS:H	1:E:488:LYS:HG2	1.55	0.44
1:E:422:PRO:HD2	1:E:504:ARG:HH22	1.82	0.44
1:G:444:PHE:O	1:G:448:ALA:HB3	2.18	0.44
1:G:564:TPO:HA	1:G:565:PRO:HD3	1.91	0.44
1:E:419:TYR:CD1	1:E:419:TYR:N	2.86	0.43
1:G:436:TRP:NE1	1:G:506:GLY:O	2.51	0.43
1:E:493:LEU:O	1:E:497:LEU:HB2	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:517:GLN:O	1:E:523:ARG:HA	2.18	0.43
1:G:293:ASP:O	1:G:296:ILE:HG22	2.18	0.43
1:G:386:LEU:HD23	1:G:392:ILE:HG22	1.99	0.43
1:A:316:VAL:N	1:A:397:TYR:HH	2.16	0.43
1:A:349:LYS:HB2	1:A:349:LYS:HE2	1.75	0.43
1:C:496:PHE:HZ	1:C:516:ILE:HD11	1.83	0.43
1:E:422:PRO:HG2	1:E:499:LYS:HA	2.00	0.43
1:E:532:GLN:HB2	1:E:534:GLN:HG3	1.99	0.43
1:E:385:LEU:O	1:E:392:ILE:HA	2.18	0.43
1:A:318:LEU:HD12	1:A:331:VAL:O	2.18	0.43
1:G:432:PHE:CD2	1:G:432:PHE:N	2.85	0.43
1:A:260:ILE:HG23	2:A:601:AFU:CAU	2.49	0.43
1:A:387:ASP:OD1	1:A:391:HIS:N	2.48	0.43
1:E:471:PHE:CD1	1:E:471:PHE:N	2.87	0.43
1:A:315:LEU:HB3	1:A:397:TYR:OH	2.19	0.43
1:C:358:TYR:HD2	1:C:446:MET:CE	2.32	0.43
1:E:305:VAL:HG22	1:E:374:ILE:CD1	2.48	0.43
1:G:296:ILE:HG23	1:G:297:ASP:OD2	2.18	0.43
1:G:370:HIS:CD2	1:G:432:PHE:HB3	2.53	0.43
1:G:375:ILE:O	1:G:400:CYS:HA	2.19	0.43
1:C:437:TRP:HZ2	1:C:453:PHE:CZ	2.37	0.42
1:A:258:ARG:NE	1:E:587:PRO:HG2	2.34	0.42
1:A:441:VAL:O	1:A:445:GLU:HG3	2.19	0.42
1:C:287:LYS:CB	1:C:574:ILE:HD12	2.50	0.42
1:C:290:VAL:HG11	1:C:299:VAL:CG1	2.49	0.42
1:A:453:PHE:CZ	1:A:474:ILE:HG12	2.54	0.42
1:G:433:SER:HB2	1:G:507:CYS:SG	2.59	0.42
1:A:381:LEU:HD12	1:A:442:LEU:CD1	2.43	0.42
1:C:491:SER:O	1:C:495:SER:OG	2.27	0.42
1:E:385:LEU:HD23	1:E:385:LEU:HA	1.83	0.42
1:G:375:ILE:HG23	1:G:435:ASP:OD2	2.19	0.42
1:G:391:HIS:HE1	1:G:537:PRO:HG3	1.84	0.42
1:G:443:MET:HE3	1:G:443:MET:HB3	1.90	0.42
1:C:412:TPO:N	1:C:430:TYR:HE2	2.17	0.42
1:C:326:SER:HA	1:C:571:VAL:HG23	2.00	0.42
1:C:374:ILE:HA	1:C:401:LYS:O	2.19	0.42
1:A:340:LEU:HG	1:A:384:VAL:HG21	2.02	0.42
1:C:269:LEU:HD12	1:C:269:LEU:C	2.40	0.42
1:G:271:VAL:HG11	1:G:282:MET:SD	2.60	0.42
1:G:357:PHE:HD1	1:G:530:MET:HE2	1.84	0.42
1:A:290:VAL:HG23	1:A:579:PHE:HZ	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:357:PHE:CD2	1:E:538:PRO:HD3	2.55	0.42
1:E:399:MET:HG2	1:E:414:CYS:HB2	2.02	0.42
1:G:384:VAL:HG12	1:G:394:LEU:HD23	2.02	0.42
1:C:269:LEU:HD12	1:C:282:MET:HB3	2.01	0.42
1:E:312:HIS:HB3	1:E:315:LEU:HD12	2.02	0.42
1:G:386:LEU:HA	1:G:391:HIS:O	2.19	0.41
1:A:319:HIS:CD2	1:C:587:PRO:HG2	2.55	0.41
1:E:334:TYR:CZ	1:E:547:PHE:O	2.74	0.41
1:A:336:ASN:CG	1:A:388:SER:HB3	2.41	0.41
1:A:385:LEU:O	1:A:393:LYS:N	2.48	0.41
1:E:256:LEU:HD13	1:E:269:LEU:CD1	2.49	0.41
1:A:387:ASP:O	1:A:541:PRO:HG3	2.20	0.41
1:C:576:GLN:HE21	1:C:576:GLN:HB3	1.61	0.41
1:E:296:ILE:HG23	1:E:297:ASP:OD2	2.20	0.41
1:E:379:LEU:HD23	1:E:438:ALA:HB3	2.02	0.41
1:E:488:LYS:O	1:E:492:VAL:HG12	2.20	0.41
1:G:419:TYR:CD2	1:G:441:VAL:HB	2.56	0.41
1:G:519:HIS:CD2	1:G:520:PRO:HD2	2.54	0.41
1:A:260:ILE:N	1:A:268:VAL:O	2.49	0.41
1:A:284:VAL:HG11	1:A:327:ARG:HD3	2.02	0.41
1:A:291:ASN:HB2	1:A:579:PHE:CZ	2.56	0.41
1:C:548:GLY:O	1:C:552:PHE:HE1	2.03	0.41
1:E:532:GLN:HG3	1:E:534:GLN:HE21	1.86	0.41
1:A:257:LEU:HD23	1:A:547:PHE:CE2	2.55	0.41
1:A:339:ASP:HB3	1:A:552:PHE:HE2	1.85	0.41
1:C:335:VAL:O	1:C:552:PHE:CZ	2.74	0.41
2:C:601:AFU:OAJ	2:C:601:AFU:CAD	2.66	0.41
1:E:260:ILE:HG21	2:E:601:AFU:CAV	2.51	0.41
1:E:421:ALA:HB3	1:E:434:VAL:HG12	2.02	0.41
1:E:436:TRP:NE1	1:E:506:GLY:O	2.53	0.41
1:C:305:VAL:HG22	1:C:374:ILE:HG21	2.02	0.41
1:A:288:GLU:HG3	1:A:289:LEU:HD12	2.03	0.41
1:A:375:ILE:HD12	1:A:401:LYS:HE2	2.03	0.41
1:C:423:GLU:CD	1:C:504:ARG:HH22	2.24	0.41
1:C:439:LEU:O	1:C:443:MET:N	2.33	0.41
1:A:383:ASN:CA	1:A:395:THR:HG22	2.51	0.40
1:A:551:ASN:OD1	1:A:551:ASN:N	2.54	0.40
1:C:298:TRP:CD1	1:C:298:TRP:C	2.95	0.40
1:C:423:GLU:CD	1:C:423:GLU:H	2.16	0.40
1:A:271:VAL:HG11	1:A:282:MET:SD	2.62	0.40
1:G:290:VAL:HG23	1:G:579:PHE:HZ	1.86	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:E:508:HIS:HA	1:E:509:PRO:HD3	1.92	0.40
1:G:344:MET:O	1:G:348:ARG:HA	2.20	0.40
1:G:517:GLN:HG2	1:G:527:TRP:CZ2	2.57	0.40
1:A:354:HIS:NE2	1:A:538:PRO:HB2	2.36	0.40
1:C:500:ASP:OD1	1:C:501:PRO:HD2	2.22	0.40
1:E:422:PRO:HD2	1:E:504:ARG:NH2	2.37	0.40
1:G:423:GLU:CD	1:G:423:GLU:H	2.25	0.40
1:G:578:GLU:H	1:G:578:GLU:HG2	1.72	0.40

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	312/345 (90%)	300 (96%)	10 (3%)	2 (1%)	25	59
1	C	307/345 (89%)	293 (95%)	12 (4%)	2 (1%)	22	56
1	E	306/345 (89%)	296 (97%)	10 (3%)	0	100	100
1	G	303/345 (88%)	287 (95%)	15 (5%)	1 (0%)	41	72
All	All	1228/1380 (89%)	1176 (96%)	47 (4%)	5 (0%)	34	67

All (5) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	405	ARG
1	C	377	ARG
1	G	405	ARG
1	A	546	GLU
1	C	541	PRO

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all X-ray entries followed by that with respect to entries of similar resolution.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	242/306 (79%)	226 (93%)	16 (7%)	16	45
1	C	227/306 (74%)	215 (95%)	12 (5%)	22	53
1	E	226/306 (74%)	208 (92%)	18 (8%)	12	37
1	G	229/306 (75%)	216 (94%)	13 (6%)	20	51
All	All	924/1224 (76%)	865 (94%)	59 (6%)	17	47

All (59) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	258	ARG
1	A	306	PHE
1	A	320	SER
1	A	327	ARG
1	A	341	MET
1	A	382	ASP
1	A	401	LYS
1	A	444	PHE
1	A	450	ARG
1	A	477	LYS
1	A	496	PHE
1	A	523	ARG
1	A	524	ASN
1	A	526	ASP
1	A	539	PHE
1	A	552	PHE
1	C	282	MET
1	C	306	PHE
1	C	311	ASN
1	C	334	TYR
1	C	344	MET
1	C	346	ARG
1	C	382	ASP
1	C	401	LYS

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Mol	Chain	Res	Type
1	C	453	PHE
1	C	513	PHE
1	C	539	PHE
1	C	553	ASP
1	E	258	ARG
1	E	269	LEU
1	E	298	TRP
1	E	336	ASN
1	E	356	ARG
1	E	357	PHE
1	E	372	ARG
1	E	413	PHE
1	E	414	CYS
1	E	480	ARG
1	E	496	PHE
1	E	513	PHE
1	E	523	ARG
1	E	530	MET
1	E	552	PHE
1	E	555	GLN
1	E	568	ASP
1	E	582	PHE
1	G	303	LYS
1	G	306	PHE
1	G	354	HIS
1	G	391	HIS
1	G	414	CYS
1	G	453	PHE
1	G	496	PHE
1	G	502	LYS
1	G	513	PHE
1	G	529	MET
1	G	539	PHE
1	G	553	ASP
1	G	582	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (8) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	323	GLN
1	C	519	HIS
1	C	576	GLN

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Mol	Chain	Res	Type
1	E	534	GLN
1	E	586	ASN
1	G	418	ASN
1	G	519	HIS
1	G	534	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

8 non-standard protein/DNA/RNA residues are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#|Z| > 2	Counts	RMSZ	#|Z| > 2
1	TPO	A	412	1	8,10,11	1.71	1 (12%)	10,14,16	1.57	1 (10%)
1	TPO	E	412	1	8,10,11	1.27	0	10,14,16	2.19	1 (10%)
1	TPO	G	412	1	8,10,11	1.76	1 (12%)	10,14,16	1.76	2 (20%)
1	TPO	A	564	1	8,10,11	1.75	2 (25%)	10,14,16	1.65	2 (20%)
1	TPO	C	564	1	8,10,11	1.71	1 (12%)	10,14,16	1.60	1 (10%)
1	TPO	G	564	1	8,10,11	1.22	0	10,14,16	1.77	1 (10%)
1	TPO	E	564	1	8,10,11	1.40	1 (12%)	10,14,16	1.72	1 (10%)
1	TPO	C	412	1	8,10,11	1.27	0	10,14,16	1.72	1 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	A	412	1	-	6/9/11/13	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
1	TPO	E	412	1	-	3/9/11/13	-
1	TPO	G	412	1	-	2/9/11/13	-
1	TPO	A	564	1	-	4/9/11/13	-
1	TPO	C	564	1	-	1/9/11/13	-
1	TPO	G	564	1	-	2/9/11/13	-
1	TPO	E	564	1	-	2/9/11/13	-
1	TPO	C	412	1	-	2/9/11/13	-

All (6) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	412	TPO	P-O1P	3.66	1.62	1.50
1	A	564	TPO	P-O1P	3.60	1.62	1.50
1	C	564	TPO	P-O1P	3.58	1.62	1.50
1	G	412	TPO	P-O1P	3.55	1.62	1.50
1	E	564	TPO	P-O2P	2.95	1.66	1.54
1	A	564	TPO	P-OG1	2.03	1.63	1.59

All (10) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	412	TPO	P-OG1-CB	-6.53	103.48	123.21
1	G	564	TPO	P-OG1-CB	-4.87	108.50	123.21
1	E	564	TPO	P-OG1-CB	-4.83	108.63	123.21
1	C	412	TPO	P-OG1-CB	-4.81	108.68	123.21
1	A	412	TPO	P-OG1-CB	-4.58	109.38	123.21
1	G	412	TPO	P-OG1-CB	-4.53	109.53	123.21
1	C	564	TPO	P-OG1-CB	-4.38	109.98	123.21
1	A	564	TPO	P-OG1-CB	-4.05	110.97	123.21
1	A	564	TPO	CG2-CB-CA	-2.09	109.03	113.16
1	G	412	TPO	CG2-CB-CA	-2.05	109.11	113.16

There are no chirality outliers.

All (22) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
1	A	412	TPO	N-CA-CB-CG2
1	A	412	TPO	N-CA-CB-OG1
1	A	412	TPO	C-CA-CB-CG2
1	A	412	TPO	CA-CB-OG1-P

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Mol	Chain	Res	Type	Atoms
1	A	564	TPO	O-C-CA-CB
1	C	412	TPO	N-CA-CB-OG1
1	C	412	TPO	O-C-CA-CB
1	C	564	TPO	O-C-CA-CB
1	E	412	TPO	N-CA-CB-OG1
1	E	412	TPO	O-C-CA-CB
1	G	412	TPO	N-CA-CB-OG1
1	G	412	TPO	O-C-CA-CB
1	G	564	TPO	CB-OG1-P-O2P
1	A	412	TPO	CG2-CB-OG1-P
1	A	412	TPO	CB-OG1-P-O1P
1	A	564	TPO	CB-OG1-P-O1P
1	E	412	TPO	CB-OG1-P-O1P
1	A	564	TPO	CB-OG1-P-O2P
1	A	564	TPO	CB-OG1-P-O3P
1	E	564	TPO	CB-OG1-P-O3P
1	G	564	TPO	CB-OG1-P-O3P
1	E	564	TPO	O-C-CA-CB

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	E	412	TPO	1	0
1	G	412	TPO	1	0
1	C	564	TPO	1	0
1	G	564	TPO	1	0
1	C	412	TPO	2	0

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry ⓘ

4 ligands are modelled in this entry.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. The Z score for a bond

length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 2$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	#$|Z| > 2$	Counts	RMSZ	#$|Z| > 2$
2	AFU	A	601	-	31,31,31	1.98	8 (25%)	41,42,42	2.20	7 (17%)
2	AFU	E	601	-	31,31,31	1.92	7 (22%)	41,42,42	2.09	8 (19%)
2	AFU	C	601	-	31,31,31	2.05	8 (25%)	41,42,42	2.39	13 (31%)
2	AFU	G	601	-	31,31,31	2.07	7 (22%)	41,42,42	2.46	11 (26%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	AFU	A	601	-	-	0/16/24/24	0/4/4/4
2	AFU	E	601	-	-	0/16/24/24	0/4/4/4
2	AFU	C	601	-	-	0/16/24/24	0/4/4/4
2	AFU	G	601	-	-	0/16/24/24	0/4/4/4

All (30) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	G	601	AFU	CAI-CAH	-6.75	1.36	1.50
2	C	601	AFU	CAI-CAH	-6.19	1.37	1.50
2	A	601	AFU	CAI-CAH	-6.04	1.37	1.50
2	E	601	AFU	CAI-CAH	-5.70	1.38	1.50
2	C	601	AFU	CAQ-CAN	-5.02	1.36	1.49
2	C	601	AFU	CAI-CAK	-4.90	1.38	1.42
2	E	601	AFU	CAI-CAK	-4.71	1.39	1.42
2	A	601	AFU	CAI-CAK	-4.70	1.39	1.42
2	A	601	AFU	CAQ-CAN	-4.50	1.37	1.49
2	E	601	AFU	CAQ-CAN	-4.34	1.38	1.49
2	G	601	AFU	CAQ-CAN	-4.22	1.38	1.49
2	G	601	AFU	CAI-CAK	-4.21	1.39	1.42
2	G	601	AFU	CAE-NAG	-4.16	1.33	1.41
2	A	601	AFU	CAE-NAG	-3.91	1.33	1.41
2	C	601	AFU	CAE-NAG	-3.87	1.33	1.41
2	E	601	AFU	CAE-NAG	-3.70	1.34	1.41
2	G	601	AFU	CAM-NAL	3.31	1.41	1.34
2	E	601	AFU	CAM-NAL	2.85	1.40	1.34
2	A	601	AFU	CAM-NAL	2.77	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	E	601	AFU	CAC-NAB	2.56	1.41	1.33
2	C	601	AFU	CAA-NAB	2.55	1.41	1.33
2	G	601	AFU	CAA-NAB	2.55	1.41	1.33
2	A	601	AFU	CAC-NAB	2.42	1.40	1.33
2	C	601	AFU	CAU-NAW	-2.41	1.32	1.38
2	A	601	AFU	CAA-NAB	2.40	1.40	1.33
2	C	601	AFU	CAM-NAL	2.34	1.39	1.34
2	G	601	AFU	CAC-NAB	2.33	1.40	1.33
2	E	601	AFU	CAA-NAB	2.24	1.40	1.33
2	A	601	AFU	CAU-NAW	-2.22	1.32	1.38
2	C	601	AFU	CAC-NAB	2.18	1.40	1.33

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	G	601	AFU	CAK-CAI-CAH	9.64	124.29	120.67
2	E	601	AFU	CAI-CAK-NAP	-9.62	115.50	122.52
2	A	601	AFU	CAI-CAK-NAP	-8.90	116.02	122.52
2	C	601	AFU	CAI-CAK-NAP	-8.50	116.32	122.52
2	G	601	AFU	CAI-CAK-NAP	-7.66	116.93	122.52
2	C	601	AFU	CAO-CAN-CAM	5.66	122.72	117.11
2	A	601	AFU	CAK-CAI-CAH	-4.76	118.89	120.67
2	C	601	AFU	CAK-CAI-CAH	-4.31	119.05	120.67
2	C	601	AFU	CAV-CAU-NAW	-4.13	116.89	121.33
2	A	601	AFU	CAO-CAN-CAM	4.03	121.11	117.11
2	A	601	AFU	CAV-CAU-NAW	-3.65	117.41	121.33
2	C	601	AFU	CAN-CAM-NAL	-3.60	118.39	124.32
2	E	601	AFU	CAO-CAN-CAM	3.56	120.64	117.11
2	G	601	AFU	CAT-CAU-NAW	-3.22	116.94	121.38
2	G	601	AFU	CAO-CAN-CAM	3.15	120.23	117.11
2	E	601	AFU	CAN-CAM-NAL	-3.10	119.22	124.32
2	A	601	AFU	CAN-CAM-NAL	-2.86	119.61	124.32
2	G	601	AFU	CAN-CAM-NAL	-2.78	119.74	124.32
2	G	601	AFU	CAR-CAQ-CAN	-2.61	116.83	121.36
2	C	601	AFU	CAR-CAQ-CAV	2.61	121.85	118.16
2	G	601	AFU	CAI-CAH-NAG	-2.61	111.09	116.06
2	C	601	AFU	CAD-CAC-NAB	-2.61	119.08	123.62
2	E	601	AFU	CAI-CAH-NAG	-2.58	111.14	116.06
2	G	601	AFU	CAX-NAW-CAU	2.56	125.01	118.09
2	E	601	AFU	CAO-CAN-CAQ	-2.55	116.64	120.86
2	C	601	AFU	CAO-CAN-CAQ	-2.51	116.70	120.86
2	C	601	AFU	CAI-CAO-CAN	-2.51	116.24	120.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	G	601	AFU	CBA-NAZ-CAY	-2.42	103.39	110.34
2	C	601	AFU	CAQ-CAV-CAU	-2.40	117.97	120.58
2	G	601	AFU	CAF-CAA-NAB	-2.25	119.71	123.62
2	E	601	AFU	OAJ-CAH-NAG	2.22	128.78	123.71
2	E	601	AFU	CAF-CAA-NAB	-2.21	119.77	123.62
2	A	601	AFU	CAD-CAC-NAB	-2.20	119.78	123.62
2	C	601	AFU	CAC-CAD-CAE	2.13	121.85	118.93
2	A	601	AFU	OAJ-CAH-NAG	2.13	128.57	123.71
2	C	601	AFU	OAJ-CAH-NAG	2.09	128.49	123.71
2	G	601	AFU	CAV-CAU-NAW	2.09	123.58	121.33
2	C	601	AFU	CAF-CAA-NAB	-2.09	119.99	123.62
2	E	601	AFU	NAP-CAK-NAL	2.02	122.78	118.35

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

4 monomers are involved in 9 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	601	AFU	2	0
2	E	601	AFU	2	0
2	C	601	AFU	3	0
2	G	601	AFU	2	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

Ligand AFU A 601

Bond lengths

Bond angles

Torsions

Rings

Ligand AFU E 601

Bond lengths

Bond angles

Torsions

Rings

Ligand AFU C 601

Bond lengths

Bond angles

Torsions

Rings

Ligand AFU G 601
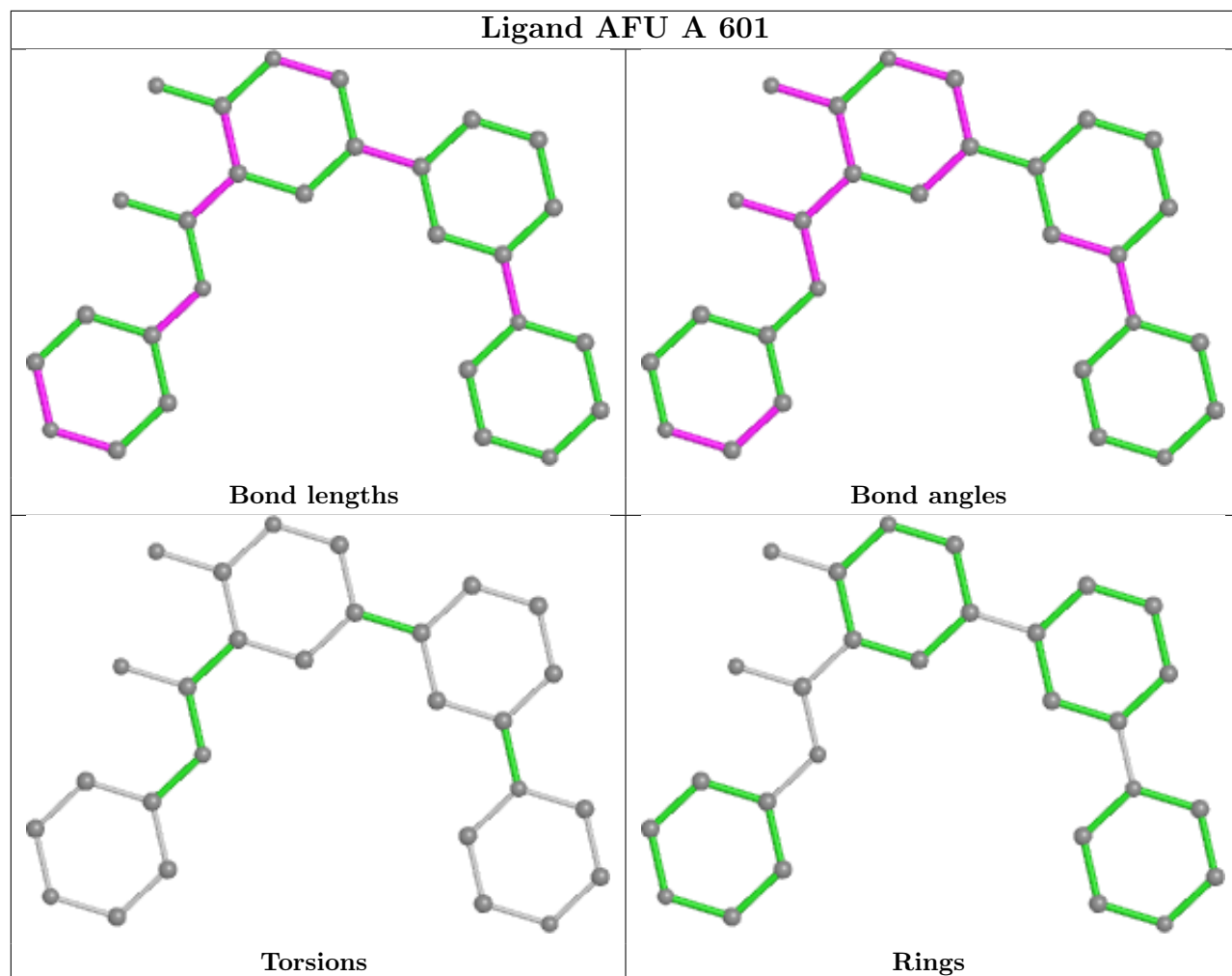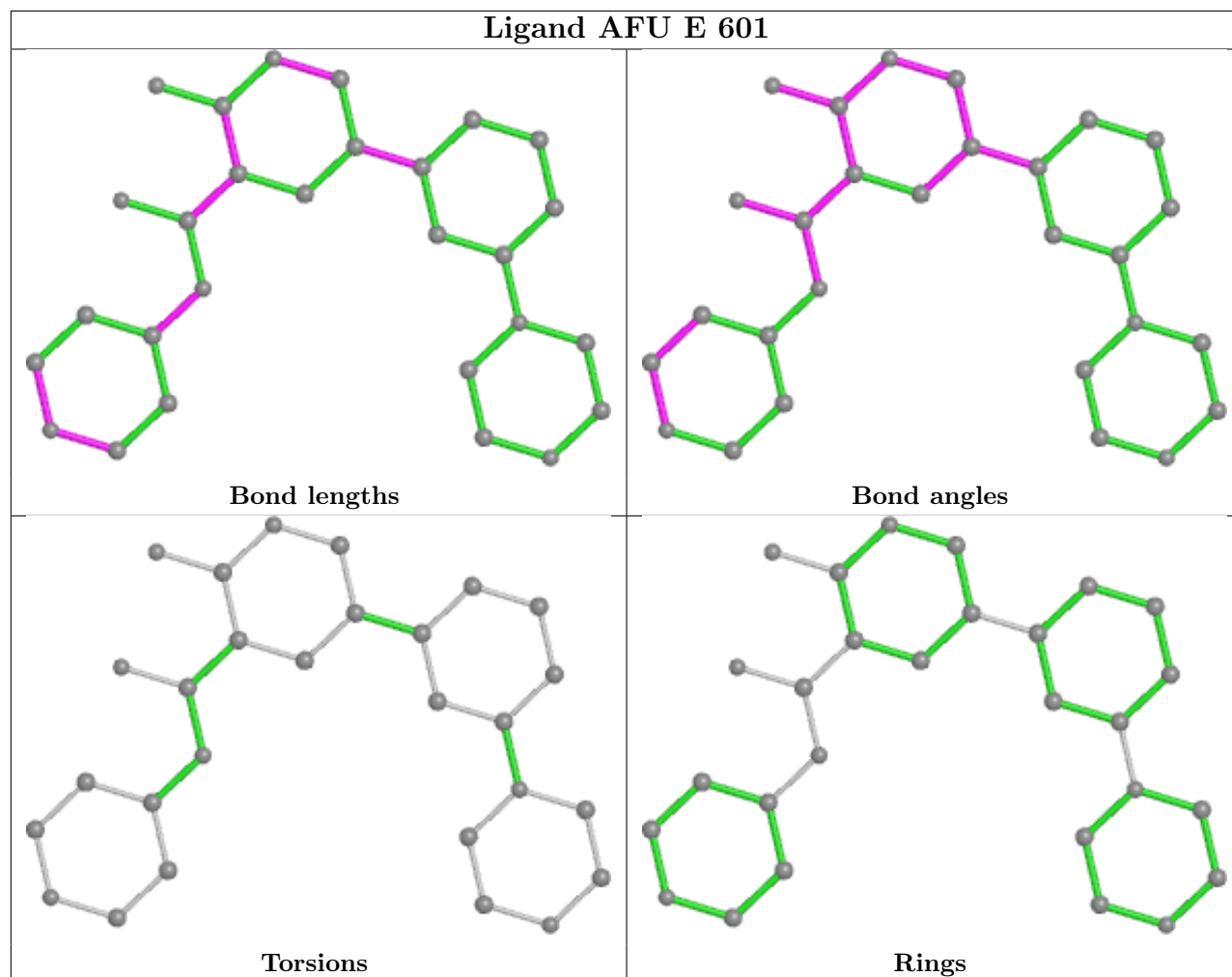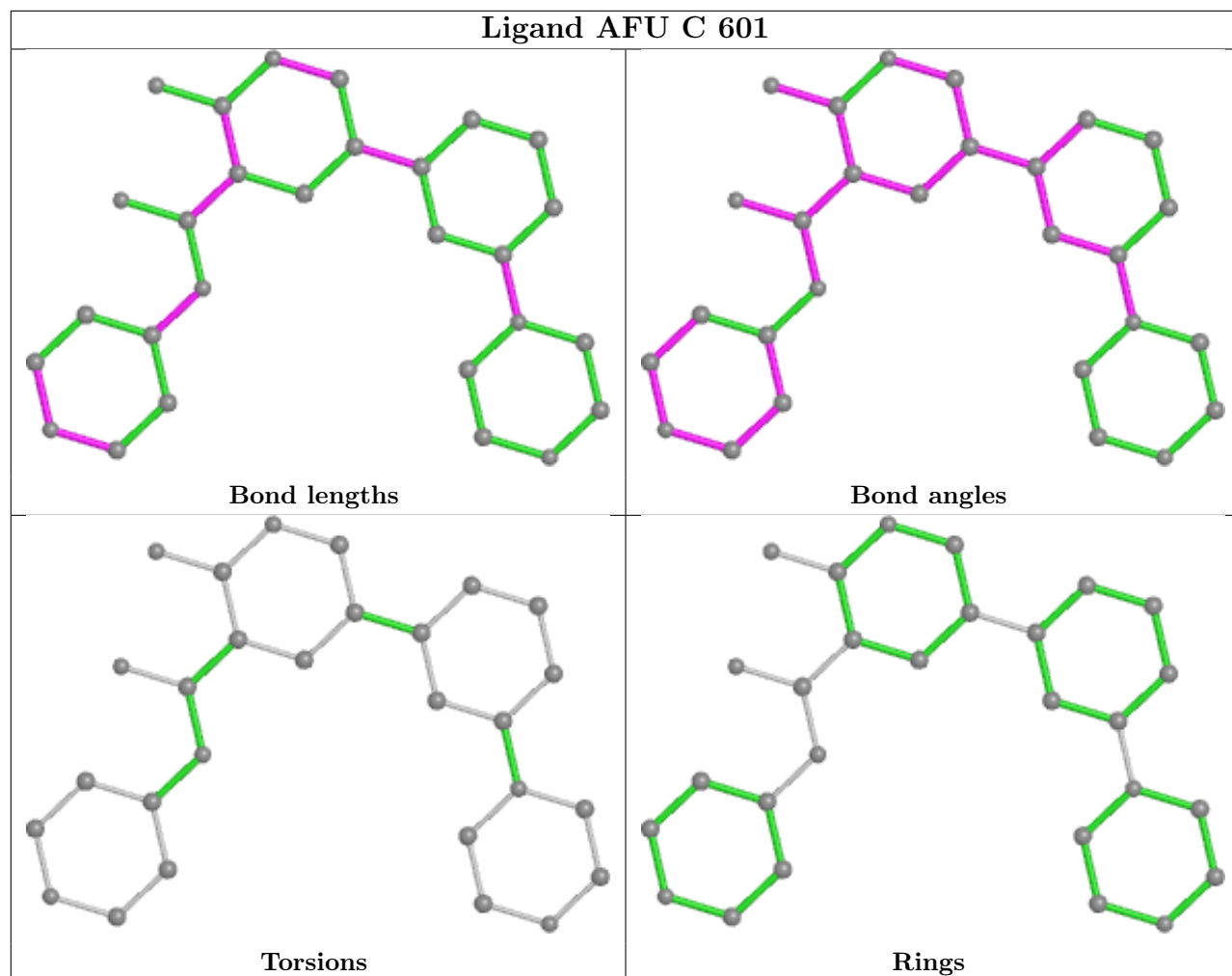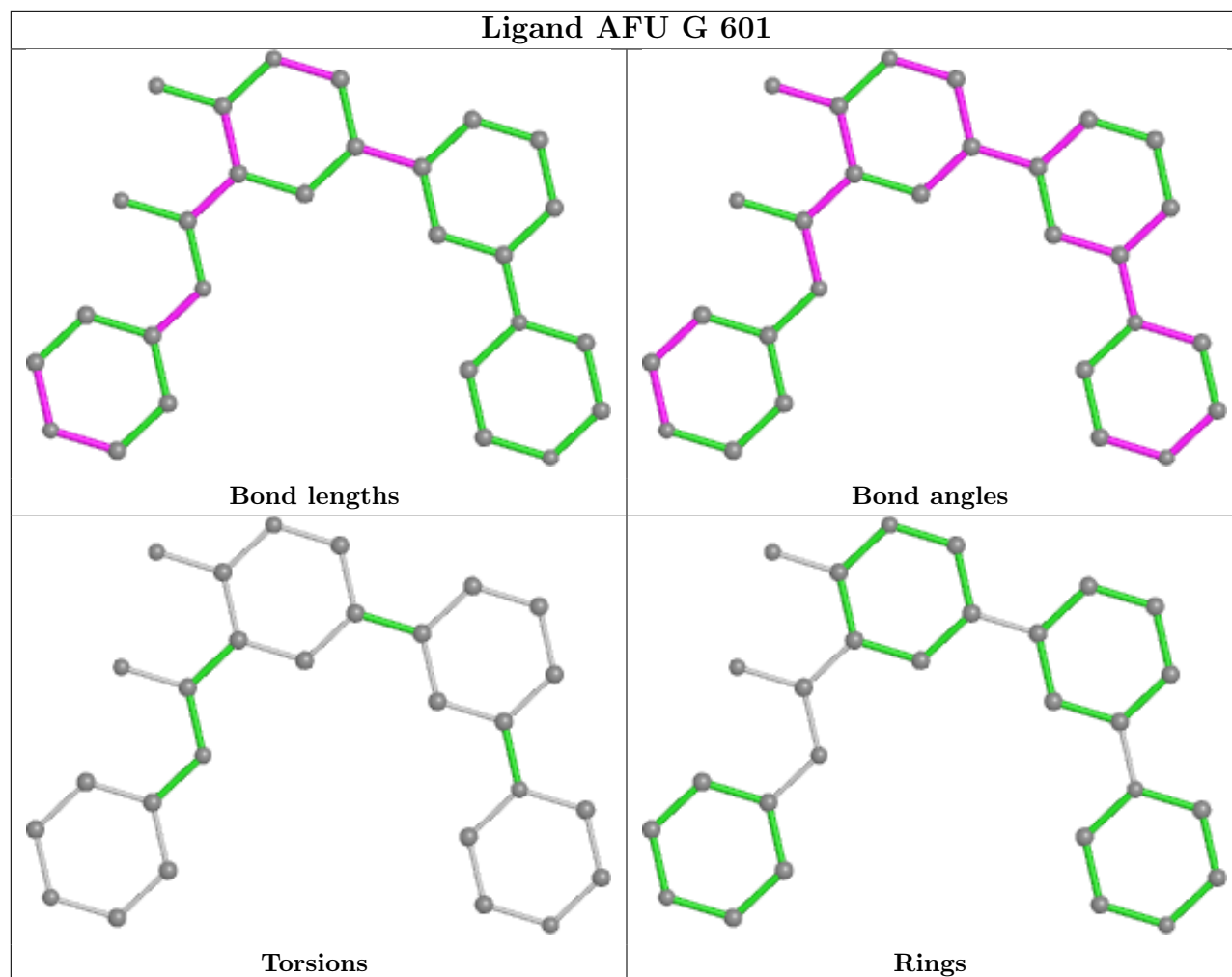
5.7 Other polymers ⓘ

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

6 Fit of model and data ⓘ

6.1 Protein, DNA and RNA chains ⓘ

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95th percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å²)	Q<0.9
1	A	318/345 (92%)	0.45	12 (3%)	40	37	22, 26, 35, 38	0
1	C	315/345 (91%)	0.42	9 (2%)	51	50	23, 31, 40, 46	0
1	E	314/345 (91%)	0.65	16 (5%)	28	26	27, 37, 47, 52	0
1	G	313/345 (90%)	0.60	18 (5%)	23	22	27, 34, 40, 46	0
All	All	1260/1380 (91%)	0.53	55 (4%)	34	32	22, 33, 43, 52	0

All (55) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	E	431	GLY	4.0
1	C	264	SER	4.0
1	E	551	ASN	3.8
1	G	587	PRO	3.8
1	E	454	ASP	3.7
1	E	546	GLU	3.7
1	A	580	GLU	3.6
1	A	557	THR	3.6
1	E	476	GLU	3.5
1	A	542	ASN	3.4
1	E	586	ASN	3.4
1	G	271	VAL	3.4
1	E	424	ILE	3.2
1	A	556	PHE	3.1
1	E	547	PHE	3.1
1	G	553	ASP	2.9
1	G	522	PHE	2.9
1	C	417	PRO	2.8
1	G	560	PRO	2.8
1	E	485	LEU	2.8
1	C	558	ASN	2.7

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Mol	Chain	Res	Type	RSRZ
1	C	545	GLY	2.7
1	A	553	ASP	2.6
1	A	558	ASN	2.6
1	G	319	HIS	2.6
1	C	554	SER	2.6
1	G	554	SER	2.5
1	G	417	PRO	2.4
1	E	378	ASP	2.4
1	E	382	ASP	2.4
1	E	354	HIS	2.4
1	G	403	GLY	2.4
1	A	522	PHE	2.3
1	G	382	ASP	2.3
1	G	301	THR	2.3
1	E	479	ILE	2.3
1	A	339	ASP	2.2
1	A	455	ILE	2.2
1	A	300	GLN	2.2
1	E	256	LEU	2.2
1	A	382	ASP	2.2
1	E	480	ARG	2.2
1	C	516	ILE	2.2
1	G	263	GLY	2.2
1	C	467	GLU	2.2
1	G	277	ASP	2.1
1	G	320	SER	2.1
1	G	454	ASP	2.1
1	G	527	TRP	2.1
1	C	569	ASP	2.1
1	A	429	ASP	2.1
1	C	528	ASP	2.1
1	G	448	ALA	2.0
1	G	568	ASP	2.0
1	E	481	ILE	2.0

## 6.2 Non-standard residues in protein, DNA, RNA chains (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
1	TPO	C	412	11/12	0.67	0.36	38,39,40,40	0
1	TPO	C	564	11/12	0.77	0.26	41,43,44,44	0
1	TPO	G	564	11/12	0.80	0.21	36,37,37,37	0
1	TPO	G	412	11/12	0.84	0.18	33,34,34,35	0
1	TPO	A	564	11/12	0.85	0.21	28,31,32,32	0
1	TPO	E	412	11/12	0.86	0.24	39,40,40,41	0
1	TPO	E	564	11/12	0.86	0.23	41,42,43,43	0
1	TPO	A	412	11/12	0.88	0.27	33,34,35,35	0

6.3 Carbohydrates ⓘ

There are no monosaccharides in this entry.

6.4 Ligands ⓘ

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. The B-factors column lists the minimum, median, 95th percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors(Å²)	Q<0.9
2	AFU	E	601	28/28	0.82	0.35	36,38,43,43	0
2	AFU	G	601	28/28	0.82	0.36	31,33,40,41	0
2	AFU	C	601	28/28	0.87	0.34	25,26,28,28	0
2	AFU	A	601	28/28	0.88	0.33	24,24,25,25	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.
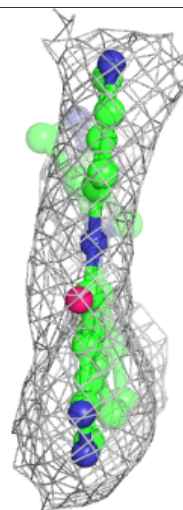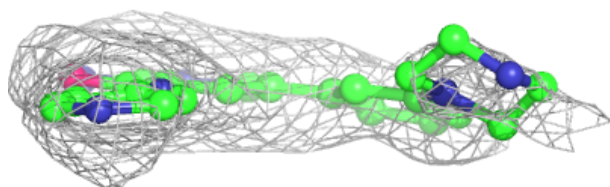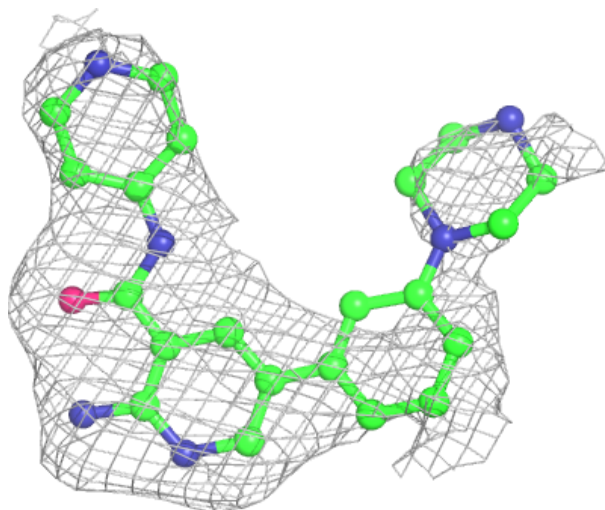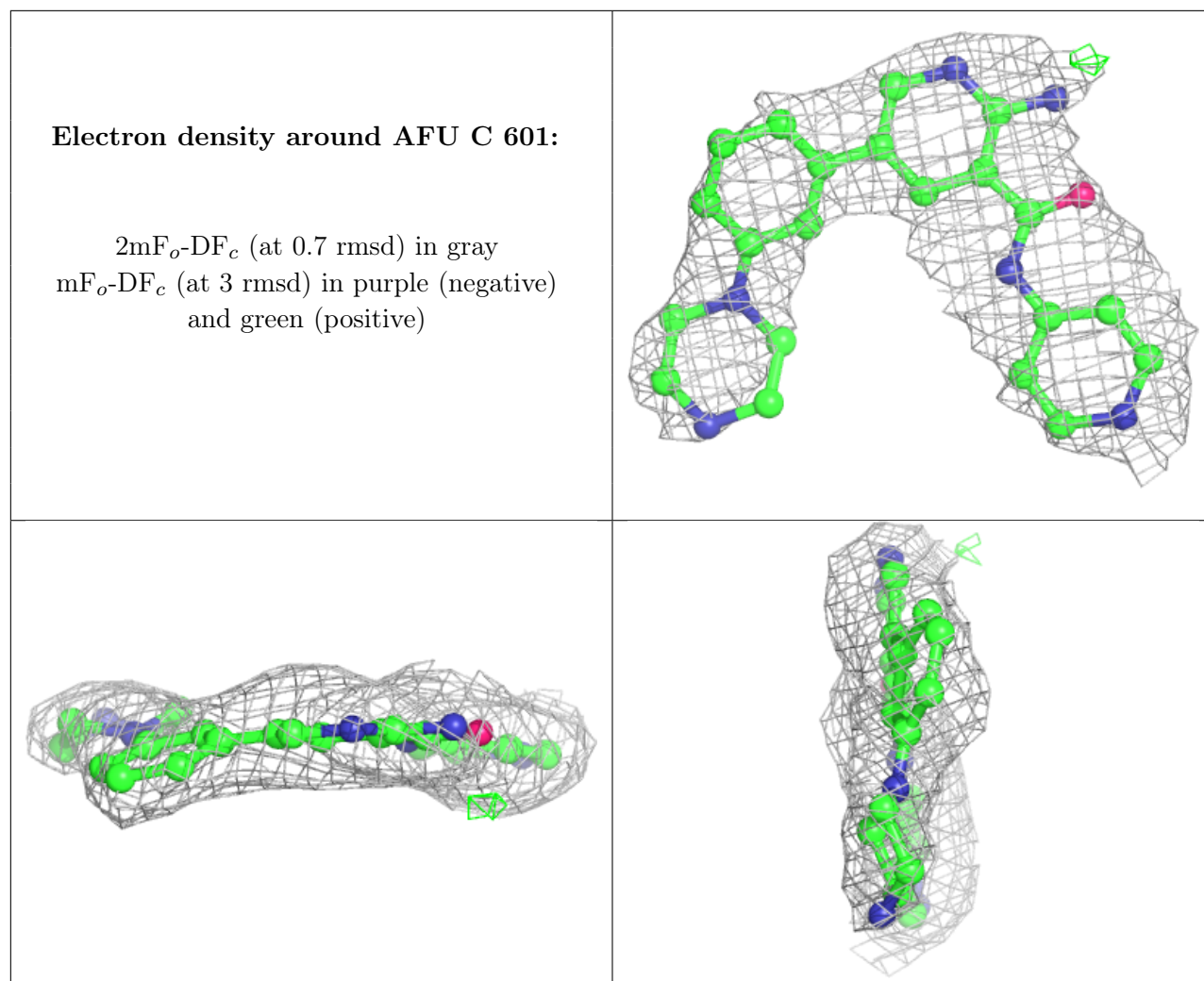
Electron density around AFU E 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
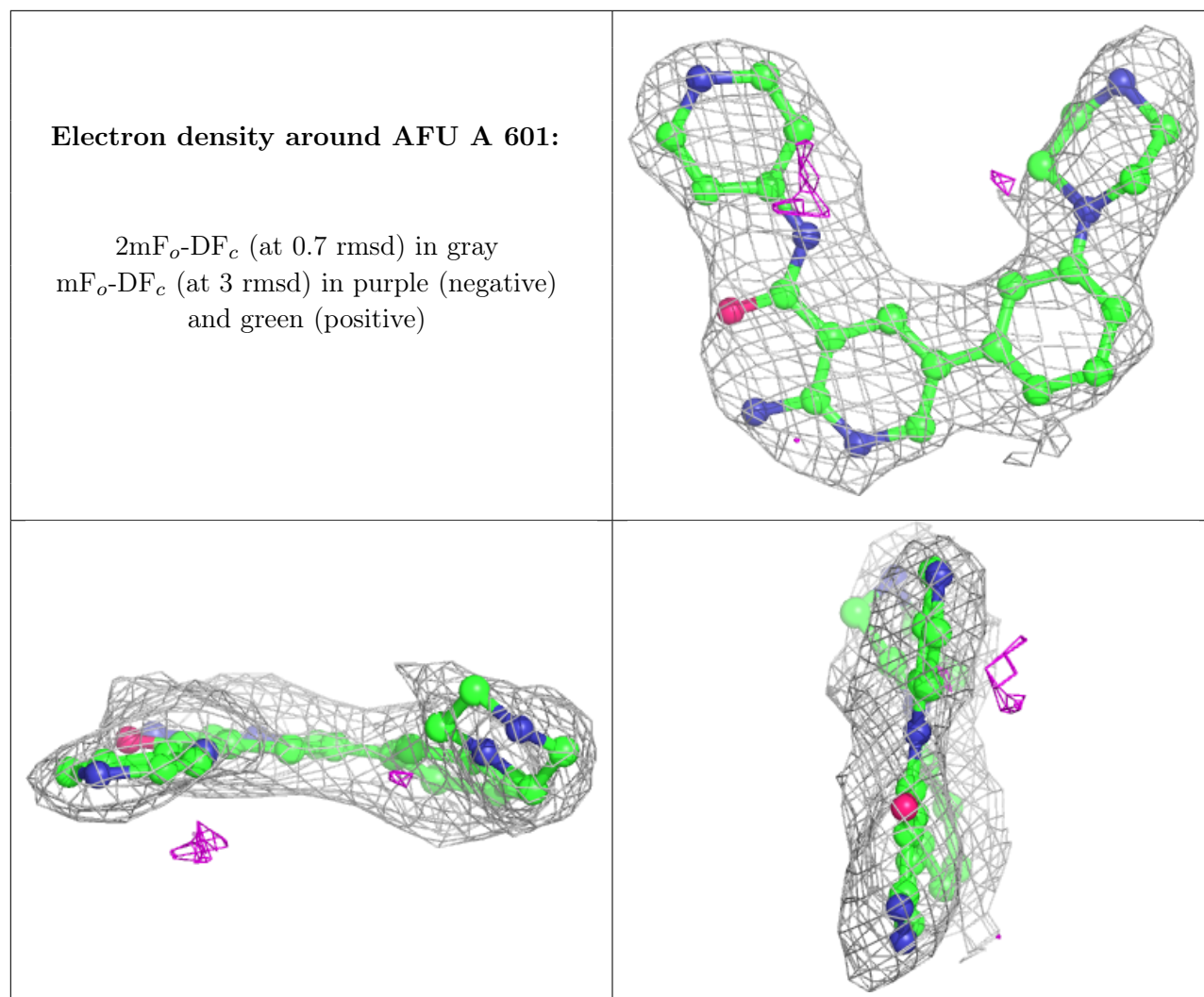mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)
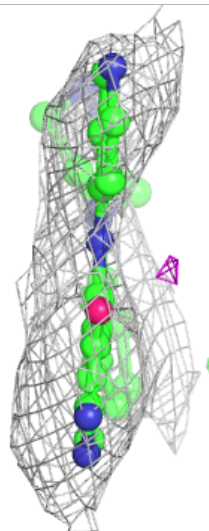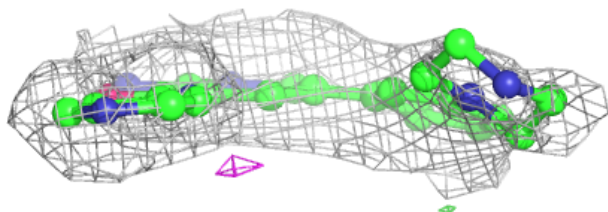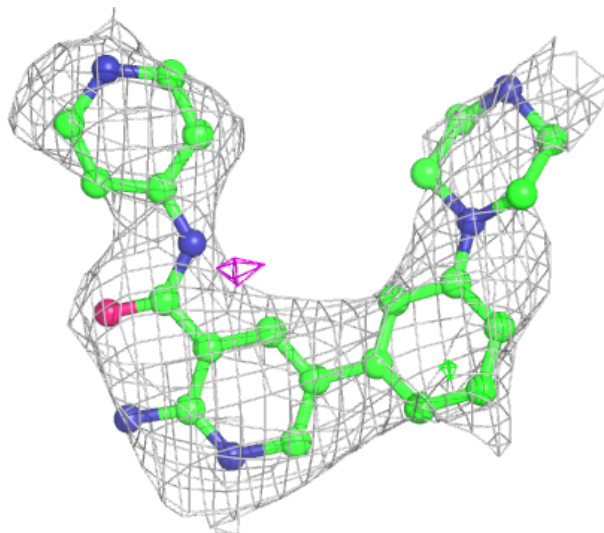
Electron density around AFU G 601:

$2mF_o$-DF_c (at 0.7 rmsd) in gray
mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around AFU C 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

Electron density around AFU A 601:

$2mF_o\text{-}DF_c$ (at 0.7 rmsd) in gray
$mF_o\text{-}DF_c$ (at 3 rmsd) in purple (negative)
and green (positive)

6.5 Other polymers ⓘ

There are no such residues in this entry.